Diethyl butanedioate
123-25-1 | DTXSID2038732

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -13.4 °C

Global applicability domain: Inside

Local applicability domain index: 9.82e-01

Confidence level: 6.60e-01

Nearest Neighbors from the Training Set

Image not found
Diethyl butanedioate
Measured: -21.0
Predicted: -13.4

Image not found
Dipropyl oxalate
Measured: -44.3
Predicted: -15.7

Image not found
Dimethyl adipate
Measured: 10.3
Predicted: -9.04

Image not found
Pentanedioic acid, diethyl ester
Measured: -24.1
Predicted: -20.9